

# $Z_2$ topological number of local quantum clusters in the orthogonal dimer model

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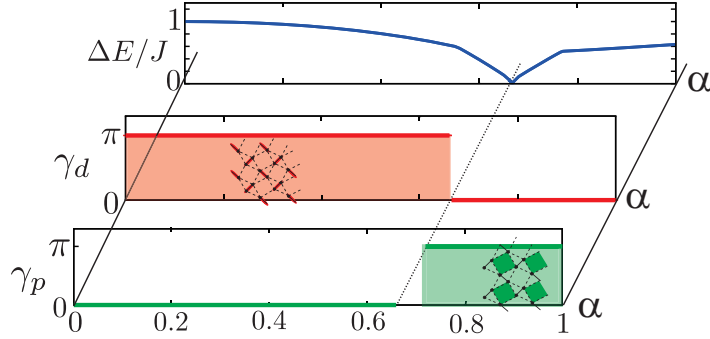
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**Abstract.** We have studied the  $Z_2$  topological number defined by the Berry phase for the gapped frustrated systems including the orthogonal dimer model which has a direct product state of local quantum clusters as the exact ground state. The  $Z_2$  topological number can clarify what kind of the local quantum clusters is formed to lift the macroscopic degeneracy due to frustration, even when the exact ground state is unknown. As a demonstration, the dimer-singlet and plaquette-singlet phase are identified by two kinds of  $Z_2$  topological numbers in the Shastry-Sutherland model and its generalization realized experimentally as  $\text{SrCu}_2(\text{BO}_3)_2$  and  $\text{CaV}_4\text{O}_9$ .

## 1. Introduction

Macroscopic degeneracy that survives at low temperature is a key feature of frustrated materials. Approaching the absolute zero temperature, the degeneracy will be lifted to meet the third law of thermodynamics. How is the degeneracy resolved? Its answer has a rich diversity, because frustrated systems have many exotic phases that are sensitive to small change. A standard scenario is the symmetry breaking mechanism that tells us an order parameter to characterize how the degeneracy is resolved. However, recent development in condensed matter physics reveals that there are topological phases where usual order parameters do not play any fundamental roles. Instead of usual order parameters such as a magnetization, topological invariants are used to characterize the topological phases and they are linked to the presence or absence of gapless edge modes. A historical example is the quantum Hall system where the topological invariant is the Chern number that is an integer defined by the Berry connection theoretically and observed as the Hall conductance experimentally. In addition to the Chern number,  $Z_2$  topological values, i.e., the integers modulo two, have been focused in recent studies on quantum spin Hall systems[1, 2]. In such topological phases, many of them are gapped.

In some frustrated materials, gap formation is another possible scenario for lifting the macroscopic degeneracy as in the two-dimensional gapped spin system,  $\text{SrCu}_2(\text{BO}_3)_2$ [3, 4]. A discovery of  $\text{SrCu}_2(\text{BO}_3)_2$  shed a light on theoretical construction of the model Hamiltonian with an exact ground state of local spin-singlets, i.e., the Shastry-Sutherland model[5, 6]. Inspired by Majumdar's one-dimensional model[7], Shastry and Sutherland constructed the two-dimensional



**Figure 1.** Gap  $\Delta E$  and Berry phases of the Shastry-Sutherland model for system size  $N = 16$  with the adiabatic parameter  $\alpha = J'/J$ .  $J$  (and  $J'$ ) is the nearest neighbor (next nearest neighbor) interaction.  $\gamma_d$  and  $\gamma_p$  are Berry phases for the DS and PS, respectively. The detail is discussed in §3.

geometrically frustrated spin system in which the exact ground state is the dimer-singlet(DS) state which is a direct product state of local spin-singlets[5]. Unless the spin gap closes, the DS state is still the exact ground state against the particular kind of perturbation due to the orthogonality of the dimers. Such construction is common in orthogonal dimer models including three-dimensional generalization[8].

The Shastry-Sutherland model also has an gapped phase, the plaquette-singlet(PS) phase[9–11], in addition to the DS phase. Unlike the DS phase, it is difficult to obtain its exact ground state in the PS phase. In fact, Weihong *et.al.*[8] have raised a possibility that the PS phase is unstable. To clarify it, one can consider an adiabatic modification of the Hamiltonian connected to the decoupled PS Hamiltonian which has a direct product state of PSs as the exact ground state. Actually, the ground state in the PS phase is adiabatically connected to that of the decoupled PS Hamiltonian[9]. The generalized theoretical model discussed in the adiabatic connection includes the 1/5-depleted square lattice that is realized as  $\text{CaV}_4\text{O}_9$ [12, 13]. In this sense, the direct product state of local quantum objects, such as DSs and PSs, and the adiabatic modification toward decoupled Hamiltonians are not just theoretical toys.

Recently, a method to obtain a decoupled Hamiltonian is proposed, that is, the  $Z_2$  topological number defined by the Berry phase[14–18]. Unless the spin gap closes, the  $Z_2$  topological number remains invariant, i.e., topologically protected against perturbation. These situations are quite similar to the case of the Chern number. The difference is that the Chern number is integer while the  $Z_2$  topological number is quantized to the following two values: a trivial value 0 or nontrivial value  $\pi$  (mod  $2\pi$ ) due to the time reversal symmetry of the spin system. However, since the Berry phase is generally defined through the local perturbation, we can consider many kinds of the  $Z_2$  topological numbers defined by the Berry phase. The  $Z_2$  topological numbers have successfully identified the spin-singlets, plaquette-singlets, and Haldane state in the spin ladders. It can be applied to not only the spin system but also the electron system including the BCS system[18]. In addition, the itinerant singlets and the Kondo singlets are identified. Recently, we have succeeded in generalizing the  $Z_2$  Berry phase into  $Z_Q$  Berry phase with any integer  $Q$ [19].

In this paper, we apply the  $Z_2$  topological number to the Shastry-Sutherland model. Our numerical result in Fig. 1 shows that the DS and PS phase are clearly identified by two kinds of  $Z_2$  topological numbers,  $\gamma_d$  and  $\gamma_p$ , respectively. Numerical detail will be explained in §3, but here we note that the ground state in the PS phase is not a simple direct product state, while there is the simple exact ground state in the DS phase. Generally speaking, although the direct product state is not an exact ground state when small long range Heisenberg exchange interactions are considered as a perturbation for real material of  $\text{SrCu}_2(\text{BO}_3)_2$ , it will be widely accepted that the ground state in the perturbation is similar to the direct product state. The similarity is naively based on the adiabatic connection of two ground states. By using the  $Z_2$  topological classification, it is possible to discuss clear equivalence of ground states via the

adiabatic connection, as we will explain in §2. This approach is demonstrated for the generalized theoretical model including  $\text{SrCu}_2(\text{BO}_3)_2$  and  $\text{CaV}_4\text{O}_9$  in §3.

## 2. Definition of the $Z_2$ topological number for orthogonal dimer models

To describe our approach, let us start with local quantum clusters. A local quantum state  $|\psi_i\rangle$  is supposed to be the singlet ground state of a quantum local Hamiltonian  $h_i$  of an  $i$ th cluster, such as a spin-singlet, plaquette-singlet, local Kondo-singlet and dimerized electrons state. The decoupled Hamiltonian is given by  $H_0 = \sum_i h_i$  with  $[h_i, h_j] = 0$ . Due to small system-size of  $h_i$ , the energy gap  $\Delta$  generally opens above the exact ground state  $|\Psi_0\rangle = \prod_i |\psi_i\rangle$ . Although the local singlet-cluster  $|\psi_i\rangle$  is a pure quantum object and does not have a classical analogue, the direct product state  $|\Psi_0\rangle$  is a classical state in the sense that there is no quantum entanglement between the clusters. The decoupled Hamiltonian is a start point to consider both construction of the orthogonal dimer model and definition of the  $Z_2$  topological number.

To construct an orthogonal dimer model generically, we connect the decoupled Hamiltonian  $H_0$  with an interaction  $H_1$ . Introducing an adiabatic parameter  $\alpha$ , we define  $H_\alpha = (1 - \alpha)H_0 + \alpha H_1$  or  $H_\alpha = H_0 + \alpha H_1$ . To keep the direct product state  $|\Psi_0\rangle$  as the exact ground state for  $\alpha > 0$ , a condition  $H_1|\Psi_0\rangle = 0$  is required. Since we supposed  $|\psi_i\rangle$  is a singlet-state,  $H_1$  can be constructed by a total spin operator for  $i$ th cluster  $T_i^\beta = \sum_l S_{il}^\beta$  ( $\beta = x, y, z$ ) with  $T_i^\beta|\psi_i\rangle = 0$ , where  $il$  indicates the  $l$ th site in the  $i$ th cluster. The condition guarantees that the ground state of  $H_\alpha$  is the direct product state around  $\alpha = 0$  to some extent as far as the gap is non-zero.

In the orthogonal dimer model, we set the local spin 1/2 cluster  $h_i = J\mathbf{S}_{i1} \cdot \mathbf{S}_{i2}$ , with the local singlet ground state  $|\psi_i\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_{i1}|\downarrow\rangle_{i2} - |\downarrow\rangle_{i1}|\uparrow\rangle_{i2})$ . Using the total spin operator  $T_i^\beta = S_{i1}^\beta + S_{i2}^\beta$ , we can construct  $H_1 = \sum_{i,i' \neq i,l'} J'_{ii'l'} \mathbf{S}_{i'l'} \cdot (\mathbf{S}_{i1} + \mathbf{S}_{i2})$ . The coefficients  $J'_{ii'l'}$  are determined by the lattice geometry. In this construction, the orthogonality of the dimer bonds is always existing, that is, the interaction between  $i1$  and  $i'l'$  is identical to that between  $i2$  and  $i'l'$  always.  $H_1$  can be generalized to a scalar product type  $H_1 = \sum J'_{ij\beta j'\beta'} (\mathbf{S}_{j\beta} \times \mathbf{S}_{j'\beta'}) \cdot (\mathbf{S}_{i1} + \mathbf{S}_{i2})$  and more complicated types. In addition, the local quantum objects can be generalized to a plaquette singlet when we consider  $h_i = J(\mathbf{S}_{i1} \cdot \mathbf{S}_{i2} + \mathbf{S}_{i2} \cdot \mathbf{S}_{i3} + \mathbf{S}_{i3} \cdot \mathbf{S}_{i4} + \mathbf{S}_{i4} \cdot \mathbf{S}_{i1})$  with  $T_i^\beta = \sum_{l=1}^4 S_{il}^\beta = T_i^{\beta\dagger}$ . In the same manner, one can consider larger cluster singlets and generalizations to local quantum objects of bosonic or fermionic systems. Note that the Hermite condition  $H_1 = H_1^\dagger$  imposes some limitation on  $H_1$ . In the above construction, the gap  $\Delta$  of  $H_0$ , which comes from a finite-size gap of the local quantum cluster, plays an important role for the stability of the exact ground state against the adiabatic parameter  $\alpha$ .

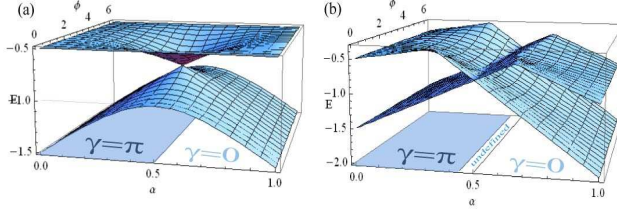
If the local ground state  $|\psi_i\rangle$  is not a singlet but a multiplet, we must deal with the macroscopic degeneracy. The gap will open above the macroscopically degenerate states and is identified by the  $Z_2$  topological number defined by non-Abelian Berry phases. Of-course, the perturbation  $H_1$  may lift the degeneracy and we need further discussion if we focus on the states below newly opened gap. In the following, we limit ourselves to a non-degenerate ground state and Abelian Berry phases in the definition of the  $Z_2$  topological number.

The Berry's geometrical phases[20] are used to calculate the macroscopic polarization in the solid with surfaces. We emphasize that an edge or surface property such as the macroscopic polarization can be obtained via the Berry phase which is calculated in the periodic bulk-system without surfaces. This is bulk-edge correspondence, which is originally proposed as the one-to-one correspondence between the Chern number defined by the Berry connections and the number of the edge states in the quantum Hall systems[21]. Such local degrees of freedom on the boundaries are also characteristic in the topological insulators, and quantum spin Hall systems[1, 2]. The bulk-edge correspondence is important for the  $Z_2$  topological number used in this paper. For example, the non-trivial  $Z_2$  topological number guarantees the existence of the Kennedy triplet for an open chain[17].

To illustrate the definition of the  $Z_2$  topological number for  $H_\alpha$ , let us consider the decoupled Hamiltonian  $H_0$  first. In our previous studies, it has been clarified that the gapped local quantum cluster, such as the spin-singlet, plaquette-singlet, and Kondo singlet, gives the non-trivial  $\pi$  Berry phase. The key ingredient to obtain the  $\pi$  Berry phase for the local cluster  $h_i$  is the unitary gauge transformation. Let us explain it with detailed definition of the Berry phase[21]. The Abelian Berry phase is defined by a local  $SU(2)$  spin twist on a specified site. When we choose a local cluster  $h_I$  and a  $l$ th site in  $h_I$ , the local spin twist is introduced by the substitution  $h_I \rightarrow h_I(\phi) = U^\dagger(\phi)h_I U(\phi)$  with  $U(\phi) = \exp[i\phi(S - S_{Il}^z)]$  for a spin  $S = 1/2$ , where  $Il$  indicates the chosen site. With using  $h_I(\phi)$ , the decoupled Hamiltonian has one-parameter dependence as  $H_0(\phi) = h_I(\phi) + \sum_{i' \neq I} h_{i'}$ . With the adiabatic parameter  $\alpha$  we define  $H_\alpha(\phi) = (1 - \alpha)H_0(\phi) + \alpha H_1$  or  $H_\alpha(\phi) = H_0(\phi) + \alpha H_1$ .

For an one-parameter dependent Hamiltonian  $H_\alpha(\phi)$ , the Berry phase  $\gamma$  is defined as  $\gamma = \int_0^{2\pi} d\phi \langle \Psi_\alpha(\phi) | \frac{d}{d\phi} | \Psi_\alpha(\phi) \rangle$ , where  $|\Psi_\alpha(\phi)\rangle$  is the ground state of  $H_\alpha(\phi)$ . The numerical integration is given by discretizing the parameter space of  $\phi$  into finite number of points[22], which is enough up to 60. The Berry phase here is quantized into 0, or  $\pi$  if the ground state is invariant under an anti-unitary operator. The anti-unitary operator is the time-reversal operator for the spin system. For the decoupled Hamiltonian  $H_0(\phi)$ , the ground state is a direct product state and has one-parameter dependence through the unitary transformation  $|\Psi_0(\phi)\rangle = U(\phi)|\Psi_0(0)\rangle$ , which gives the  $\pi$  Berry phase, because  $\gamma = 2\pi(S - \langle \Psi(0) | S_{Il}^z | \Psi(0) \rangle) = \pi$  in the spin  $S = 1/2$  case. This result does not depend on the detail of the local Hamiltonian  $h_i$ . When the Hamiltonian is  $H_\alpha(\phi) = (1 - \alpha)H_0(\phi) + \alpha H_1$ , there should be the change of the  $Z_2$  topological number. At  $\alpha = 1$ , since the Hamiltonian  $H_{\alpha=1}(\phi) = H_1$  does not depend on  $\phi$ , the Berry phase  $\gamma$  cannot become the non-trivial value  $\pi$ , that is,  $\gamma$  is zero if the gap opens or undefined if the gap closes. Then, there is inevitably the change of  $\gamma$  in the adiabatic modification via  $\alpha$ , which signals whether the ground state is equivalent to the direct product states or not. It should be noted that since  $H_\alpha(\phi) \neq U^\dagger(\phi)H_\alpha U(\phi)$  due to  $H_1$ , the Hamiltonian  $H_\alpha(\phi)$  is able to have a local flux, which cannot be gauged out. Then, the problem is non-trivial for generic  $H_1$ .

Typically, there are two types of the transitions for the  $Z_2$  Berry phase in the adiabatic modification  $\alpha$ . To discuss it, let us show an example of a local cluster, the  $N = 4$  spin  $S = 1/2$  system with the decoupled Hamiltonian  $H_0(\phi) = U^\dagger(\phi)h_1 U(\phi) + h_2$  of the dimer singlets  $h_i = \mathbf{S}_{i1} \cdot \mathbf{S}_{i2}$  and the local spin twist  $U(\phi) = \exp[i\phi(S - S_{11}^z)]$ . Here we consider two kinds of Hamiltonians  $H_\alpha(\phi) = (1 - \alpha)H_0(\phi) + \alpha H_1$ : (a) the non-orthogonal interaction  $H_1 = \mathbf{S}_{12} \cdot \mathbf{S}_{21} + \mathbf{S}_{11} \cdot \mathbf{S}_{22}$  and (b) the orthogonal interaction  $H_1 = (\mathbf{S}_{11} + \mathbf{S}_{12}) \cdot (\mathbf{S}_{21} + \mathbf{S}_{22})$ . Due to the lattice symmetry, the Berry phase does not depend on the site where  $U(\phi)$  is introduced. In the case (b), the exact ground state of  $H_\alpha(0)$  is a direct product state of the dimer singlets for  $\alpha < \alpha_c$  and there is a level cross at  $\alpha = \alpha_c = 1/2$ . On the contrary, in the case (a), the direct product state is not an exact ground state for  $\alpha > 0$  and there is finite gap without any level cross in the range of  $\alpha \in [0, 1]$  for  $H_\alpha(0)$ . We expect that in the latter adiabatic modification two DSs delocalize asymmetrically except for the symmetric point  $\alpha = \alpha_c$ . The  $Z_2$  Berry phase detects the asymmetry of the DSs. In Fig. 2, the result of the  $Z_2$  Berry phase is shown in both cases (a) and (b). In the case (a), the  $Z_2$  Berry phase clearly identified the two phases connected to the two decoupled models,  $\alpha = 0$  and 1, respectively. At the phase boundary  $\alpha = \alpha_c$ , the  $Z_2$  Berry phase becomes undefined because the level cross occurs at  $\phi = \pi$ . In other words, the diabolic point of the Dirac cone generates the  $\pi$  Berry phase. Here, we emphasize that the Hamiltonian  $H_\alpha(0)$  at  $\phi = 0$  has no gap closing in the adiabatic modification via  $\alpha$  and there is not a transition but a cross-over[18]. In the case (b) as shown in Fig. 2(b), the level cross at  $\alpha = \alpha_c$  without twist  $\phi$  induces a finite range of the undefined region of the  $Z_2$  Berry phase.



**Figure 2.** Two typical energy diagrams as a function of  $\phi$  and  $\alpha$  of  $H_\alpha(\phi) = (1 - \alpha)H_0(\phi) + \alpha H_1$  with (a) the non-orthogonal interaction  $H_1 = \mathbf{S}_{12} \cdot \mathbf{S}_{21} + \mathbf{S}_{11} \cdot \mathbf{S}_{22}$  and (b) the orthogonal interaction  $H_1 = (\mathbf{S}_{11} + \mathbf{S}_{12}) \cdot (\mathbf{S}_{21} + \mathbf{S}_{22})$ .

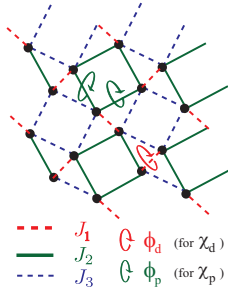
### 3. Results on the Shastry-Sutherland model

Here we discuss adiabatic modifications of the Shastry-Sutherland model as shown in Fig. 1. The Shastry-Sutherland model with  $J$  and  $J' = \alpha J$  can be defined as the case  $J_1 = J$  and  $J_2 = J_3 = J'$  of the generalized model as shown in Fig. 3. As mentioned in previous sections, the definition of the Berry phase depends on the local spin twist and on the choice of the decoupled Hamiltonian for a given Hamiltonian. For this Shastry-Sutherland model,  $\gamma_d$  (and  $\gamma_p$ ) is defined by the local spin twist  $\phi_d$  ( $\phi_p$ ) shown in Fig. 3. The decoupled DS (and PS) Hamiltonian only with  $J_1$  ( $J_2$ ) corresponds to  $\gamma_d$  ( $\gamma_p$ ). Since the Shastry-Sutherland model has the exact ground state of the DSs, the level cross at  $\alpha = \alpha_c$  is expected as in Fig. 2(b). Actually, in our calculation with the small system size  $N = 16$ , there is the first-order quantum phase transition, that is, a gap closing  $\Delta = 0$  occurs at  $\alpha_c = 0.67$  as shown in Fig. 1. Moreover,  $\gamma_d$  shows a clear transition at  $\alpha = \alpha_c$  in Fig. 1. This is quite natural because we know the exact DS ground state for  $\alpha = J'/J < \alpha_c$ . The question arising here is how the ground state for  $\alpha > \alpha_c$  is identified. To answer this question we introduce another  $Z_2$  topological number,  $\gamma_p$ , which corresponds to the decoupled PS Hamiltonian having the direct product state of local PSs as the exact ground state. Figure 1 shows that the two  $Z_2$  topological numbers can identify the DS phase for  $\alpha < \alpha_c$  and the PS phase for  $\alpha > \alpha_c$ . However, since there is the first-order phase transition at  $\alpha_c$ , the  $Z_2$  Berry phase will show instability just around the level cross point as shown in Fig. 2(b). In fact,  $\gamma_p$  shows an undefined region around  $\alpha = \alpha_c$  as shown in Fig. 1. Although the system size is too small and the transition point  $\alpha_c$  is not comparable to previous studies, the  $Z_2$  Berry phase clarifies a PS-type character of the ground state for  $\alpha > \alpha_c$ .

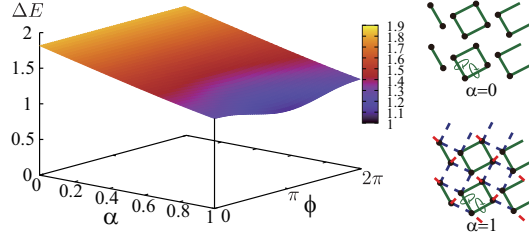
In addition, we consider  $J_2/J_1 = 1.82$  and  $J_3/J_1 = 0.95$  in the parameter space  $J_1, J_2$ , and  $J_3$  of the generalized model in Fig. 3, which corresponds to  $\text{CaV}_4\text{O}_9$  and is in the PS phase[10]. To clarify the property of the ground state by the  $Z_2$  topological number, we calculated  $\gamma_p$  and we obtained  $\gamma_p = \pi$  for  $N = 16$  sites. To illustrate the result, we show the gap  $\Delta E$  as a function of twist  $\phi = \phi_p$  and the adiabatic parameter  $\alpha$  from the decoupled PS Hamiltonian at  $\alpha = 0$  to  $\text{CaV}_4\text{O}_9$  at  $\alpha = 1$ . The decoupled PS Hamiltonian has  $\gamma_p = \pi$  by definition. Figure 4 shows that there is no gap closing in the adiabatic modification not only at  $\phi = 0$  but in whole region of  $\phi \in [0, 2\pi]$ . To change the  $Z_2$  topological number, the gap closing is required as discussed in §2. In this sense,  $\gamma_p = \pi$  means that the state is adiabatically connected to the direct product state in the two dimensional parameter space including the gauge twist angle  $\phi \in [0, 2\pi]$ .

### 4. Summary

In summary, we have studied the  $Z_2$  topological number of the orthogonal dimer model as the gapped frustrated spin system. The construction of the orthogonal dimer model with the exact ground state and the  $Z_2$  topological number  $\gamma_d$  are based on the same decoupled DS Hamiltonian. As shown in Fig. 1, the DS phase has the non-trivial  $Z_2$  topological number,  $\gamma_d = \pi$ , corresponding the direct product state of DSs. The orthogonal dimer model shows the first-order transition with a level crossing, as shown in Fig. 2(b), in the finite-size calculation. Although the exact ground state after the transition is unknown, the  $Z_2$  topological number



**Figure 3.** Hamiltonian with  $J_1$ ,  $J_2$ , and  $J_3$ .



**Figure 4.** The gap  $\Delta E$  for the  $Z_2$  topological number  $\gamma_p$ . The twist  $\phi = \phi_p$  is defined for the decoupled PS Hamiltonian with the bonds  $J_2 = 1.82$ . The adiabatic parameter  $\alpha$  is introduced as  $J_1 = \alpha, J_3 = 0.95\alpha$ .

which corresponds to the decoupled PS Hamiltonian shows  $\gamma_p = \pi$  for  $\alpha > \alpha_c$  as shown in Fig. 1 and for the specified parameter corresponding to  $\text{CaV}_4\text{O}_9$  as clarified in Fig. 4. Even though our analysis using the exact diagonalization is limited for the small system-size, this result agrees with existence of the PS phase discussed in the previous studies[9, 10].

## Acknowledgments

The authors are grateful to A. Koga for his valuable discussion. This work was supported by a Grant-in-Aid from the Ministry of Education, No. 20340098 from JSPS, No.22014002 on Priority Areas from MEXT. Some numerical calculations were carried out on Altix3700BX2 at YITP in Kyoto University and the facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

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